Combustion Technology and High-Temperature Research at the University of Pittsburgh

Overview

Combustion technology and high-temperature related research activities in the University of Pittsburgh's School of Engineering span three departments: the Department of Mechanical Engineering (ME), the Department of Materials Science and Engineering (MSE), and the Department of Chemical and Petroleum Engineering (ChE).

Within this framework, research activities range from detailed numerical simulations to experimental studies, and cover a wide spectrum of combustion-related research topics:

- Materials:
  - alloys and high-temperature coatings for solid oxide fuel cells and gas turbines (MSE)
  - nanostructured composite materials for high-temperature catalytic oxidation (ChE)
- Reactive Flows:
  - large scale numerical simulations and modeling of turbulent combustion (ME)
  - detailed reaction and reactor simulations for catalytic high-temperature reactions (ChE)
- Reactor/Burner Concepts:
  - heat-integrated reactors for efficient energy utilization (ChE)

In the panels at right, each department presents a brief overview over its current research activities related to combustion technology and high-temperature reactions, along with some highlights from recent research projects.

Mechanical Engineering

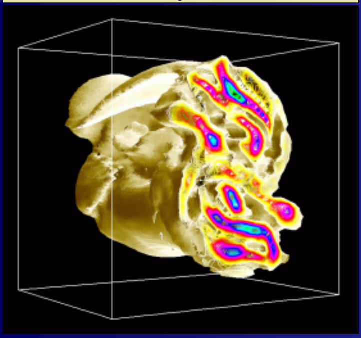
Introduction

Research in combustion is being conducted in the Department of Mechanical Engineering at the University of Pittsburgh. The emphasis of this program is on the understanding of engineering "physical" phenomena, not the development of numerical algorithms. Currently, our research is focused on combustion, propulsion, turbulence and computational fluid dynamics (CFD). Student participation is one of the most important elements of this program.

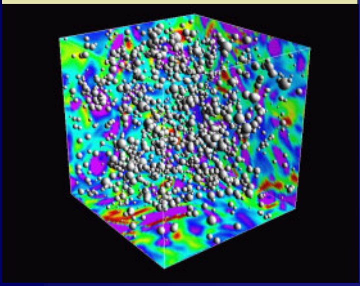
Dr. Peyman Givi is William Kepler Whiteford Chair Professor of Mechanical Engineering at the University of Pittsburgh. Previously, he held the position of University at Buffalo Distinguished Professor at the State University of New York at Buffalo. Prior to that, he was a research scientist at Flow Industries, Inc. in Seattle, and has had visiting appointments at the NASA Langley Research Center and the NASA Glenn Research Center. Dr. Givi was amongst the first 15 engineering educators nationwide to be honored with the Presidential Faculty Fellowship from President George Bush. He has also received the Young Investigator Award of the Office of Naval Research, and the Presidential Young Investigator Award of the National Science Foundation.

Sponsors: Our research has been of interest and relevance to government agencies, national laboratories and private industry. Some of our most recent sponsors include: Air Force Office of Scientific Research, American Chemical Society, Ford Motor Company, NASA Headquarters, NASA Langley Research Center, NASA Glenn Research Center, National Science Foundation, Naval Research Laboratory, Office of Naval Research, Sandia National Laboratories, and Wright Patterson Air Force Laboratories.

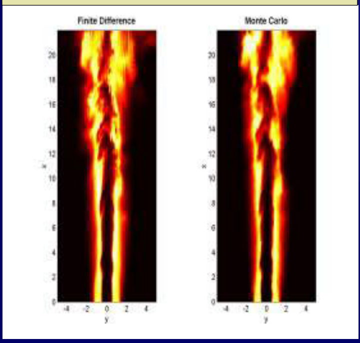
Vortex Stretching in a Temporal Mixing Layer



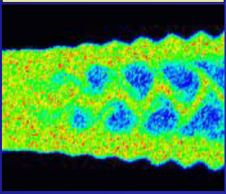
Polydispersed Evaporating Droplets in Homogeneous Turbulence



LES of Sandia Flame D

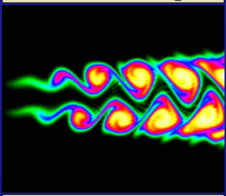


Lagrangian Simulation of the Filtered Density Function

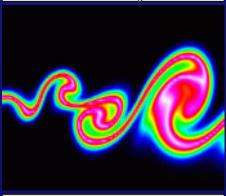


Coherent Structures in Turbulent Combustion

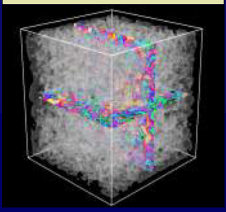
Large Eddy Simulation of a Planar Reacting Jet



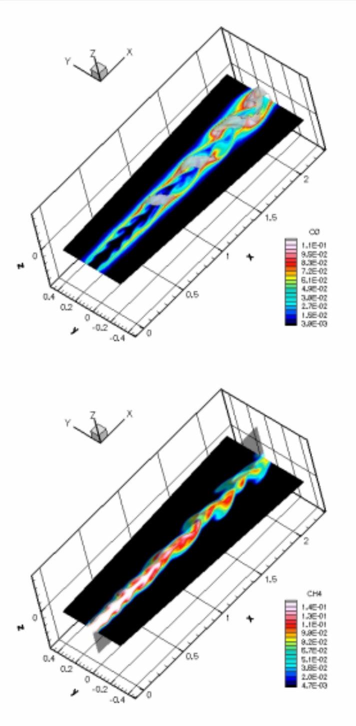
Vortical Structures in a spatially Developing Shear Layer



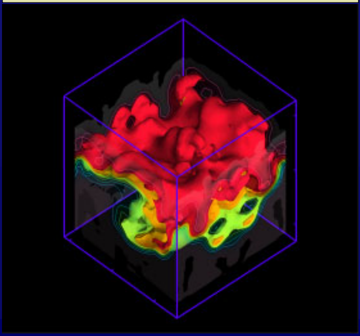
Monte Carlo Particles in Incompressible Turbulence



Spectral/hp Element Simulation of a Turbulent Reacting Jet



Flame Convolution by Turbulence



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Chemical Engineering

Introduction

High-temperature catalytic conversion of hydrocarbons by total oxidation (i.e. combustion) as well as partial oxidation (such as hydrogen or synthesis gas production) is characterized by similar challenges: the need to develop energy-efficient reactor concepts to achieve and/or handle extremely high reaction temperatures, and the demand for catalyst with improved long-term stability at these high-temperature conditions.

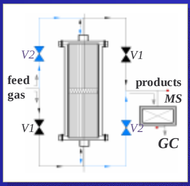
We are investigating these problems using catalytic partial oxidation of methane to synthesis gas at high-temperature (T>900°C), millisecond contact time conditions (τ = 1-50 ms) as test reaction.

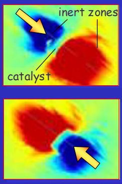
Heat-Integrated Reactor Concepts

Reverse-Flow Reactor (RFR): periodic reversal of flow direction in reactor leads to very efficient integration of regenerative heat-exchange

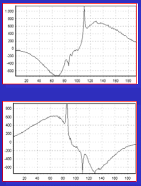
Experimental Set-Up: Computer-controlled reactor operation and data acquisition

laboratory-scale test reactor





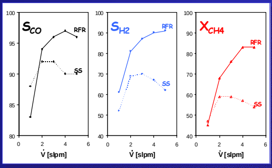
red = 'heating up'
blue = 'cooling down'

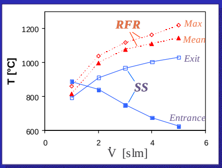


sharp peaks: (fast) reaction front
broad peaks: (slow) heat-reservoirs

Results:

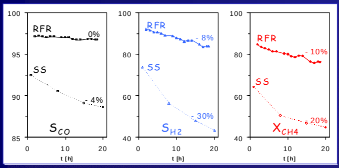
- strongly increase in syngas selectivities and methane conversion
- higher throughput (i.e. shorter residence times) possible with even further increased syngas yields





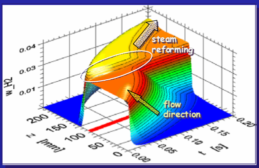
CH_4/O_2 = 2.0, $\tau/2$ = 15s

- strong catalyst deactivation intrinsically compensated by reverse-flow operation!



Detailed Reactor Simulations:

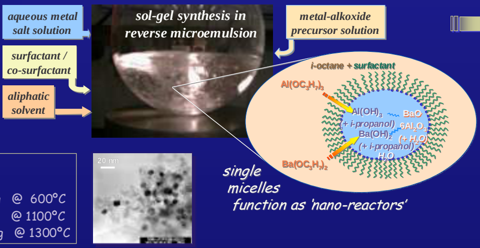
- reaction proceeds via direct oxidation mechanism
- homogeneous reaction insignificant at ultra-short residence times
- in reverse-flow operation, steam reforming after flow reversal contributes some to improved yields



Very efficient reactor concept for high-throughput (decentralized) processes leads to strong improvements in syngas yields and prolongs stable catalyst operation!

Nano-Composite Catalysts

Catalyst Synthesis:



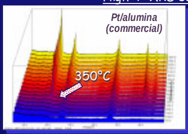
24 - 72 h aging
washing & phase separation
drying (freeze-drying)
Calcination (T=600-1300°C)

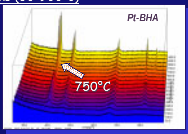
Pt-content:	5 - 10 wt%
average particle size:	5 - 15 nm
surface area (BET):	300 - 400 m²/g @ 600°C
	100 - 200 m²/g @ 1100°C
	10 - 25 m²/g @ 1300°C

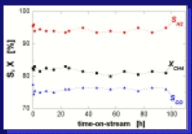
High-Temperature Stability:

unusual stabilization of nanoparticles
→ very stable catalyst activity

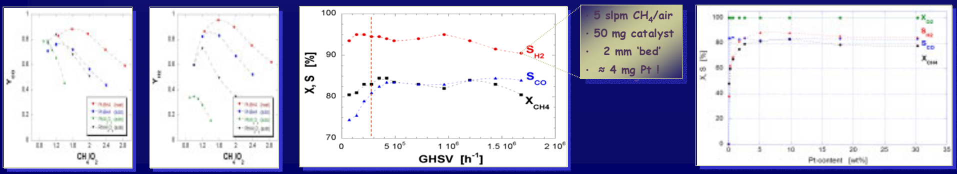
High-T XRD scans (50-900°C)







Reactive Tests:



5 slpm CH_4/air
50 mg catalyst
2 mm 'bed'
≈ 4 mg Pt !

Highly active and selective catalysts with exceptional high-temperature stability!

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Materials Science & Engineering

Fundamental Studies of the Durability of Materials for Interconnects in Solid Oxide Fuel Cells

Project Aim:

The aim of this project is to evaluate the chemical and thermomechanical stability of ferritic alloys in the fuel cell environment. The understanding gained will be used to attempt to optimize the properties of the ferritic alloys.
A parallel study is evaluating the potential use of alternate metallic materials as interconnects.

Project Tasks:

The project is divided into three tasks:

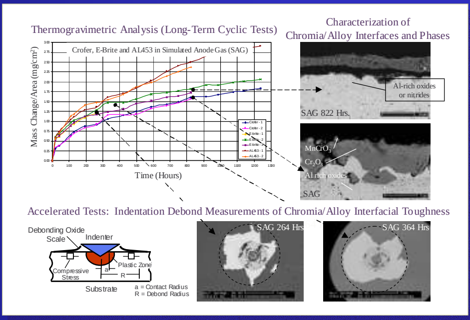
TASK I: Mechanism-Based Evaluation Procedures
- Growth Rates of Chromia Scales on Cr and Ferritic Alloys
- Adhesion of Chromia Scales
- Oxide Evaporation

TASK II: Fundamental Aspects of Thermomechanical Behavior
- XRD Stress Measurements (Chromia Films)
- Indentation Testing of Interface Adhesion
- Indentation Test Fracture Mechanics Analysis

TASK III: Alternative Material Choices
- This Task involves theoretical analysis of possible alternative metallic interconnect schemes.

Protocols for Evaluating Existing and New Interconnect Alloys:

Program Team
- Prof. F. S. Pettit, Dept. of Mat. Sci. and Eng., University of Pittsburgh (Pitt-MSE)
- Prof. G. H. Meier, Dept. of Mat. Sci. and Eng., University of Pittsburgh
- Prof. J. L. Beuth, Dept. of Mech. Eng., Carnegie Mellon University (CMU)



Mechanism-Based Testing Methodology For Improving the Oxidation, Hot Corrosion and Impact Resistance of High-Temperature Coatings for Advanced Gas Turbines

Gas Turbine Needs

In the next generation gas turbine, resistance to thermal cycling damage may be as important as resistance to long isothermal exposures. Moreover, metallic coatings and Thermal Barrier Coatings (TBCs) may encounter attack by deposits arising from combustion of low-grade fuel and air borne impurities. Finally, there is currently a need for nondestructive techniques to assess metallic coating and TBC degradation and damage as a result of exposure to cyclic oxidation and hot corrosion conditions as well as foreign object-impact damage.

Program Focus

- Development of a mechanism-based testing methodology for improving the oxidation, hot corrosion and impact resistance of high temperature metallic coatings and TBCs
- Incorporation of a significant number of nondestructive tests in this methodology directed at assessing coatings degradation and damage accumulation.

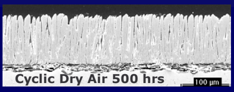
Project Approach

Leverage the talents of a multi-disciplinary, multi-organization team to achieve the project objectives.

Program Team
- Prof. F. S. Pettit, Dept. of Mat. Sci. and Eng., University of Pittsburgh (Pitt-MSE)
- Prof. G. H. Meier, Dept. of Mat. Sci. and Eng., University of Pittsburgh
- Prof. J. L. Beuth, Dept. of Mech. Eng., Carnegie Mellon University (CMU)
- Prof. S. Mao, Dept of Mech. Eng., University of Pittsburgh (Pitt-ME)
- Dr. M. Lance, Oak Ridge National Laboratory (ORNL)
- Dr. W. Ellingson, Argonne National Laboratory (ANL)
- Dr. W. E. Fuller, National Institute of Standards and Technology (NIST)
- Industrial Partners: Praxair & Howmet

Sectioned Micrograph - TBC - Isothermal, Dry Air vs. Cyclic Thermal, Dry Air, 1100°C

- Cycle-Induced Damage is Clearly Occurring
- Damage Makes Cracking in the Oxide and TBC as favorable as Interfacial Cracking



Materials and Techniques

- Substrates: Single Crystal Nickel Base Superalloys
  CMSX-4
  René N5
- Coatings: NiCoCrAlY Overlay Coatings
  Diffusion Aluminide Coatings
  TBC with NiCoCrAlY Bond coat
  TBC with Aluminide Bond Coat
- Evaluation Techniques:
  - Destructive:
    Cross-section Metallography (Pitt-MSE)
    Indentation (CMU)
  - Nondestructive:
    X-ray Stress Measurement (Pitt-MSE)
    Piezospectroscopic Stress Measurement (ORNL)
  - Elastic Optical Backscatter Imaging (ANL)
  - Impedance Spectroscopy (Pitt-ME)
  - Acoustic Emission Measurements (Pitt-MSE)
  - Modeling:
    Prediction of long-term Behavior (NIST)

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